ACCGE-17 ABSTRACT

Stability of Detached Solidification

K. Mazuruk[a], M. P. Volz[b], A. Cröll[c]

[a]University of Alabama in Huntsville, Huntsville, AL 35762, USA
[b]NASA, Marshall Space Flight Center, EM30, Huntsville, AL 35812, USA
[c]Kristallographisches Institut, University of Freiburg, Hebelstr. 25, D-79104, Freiburg, Germany

Abstract

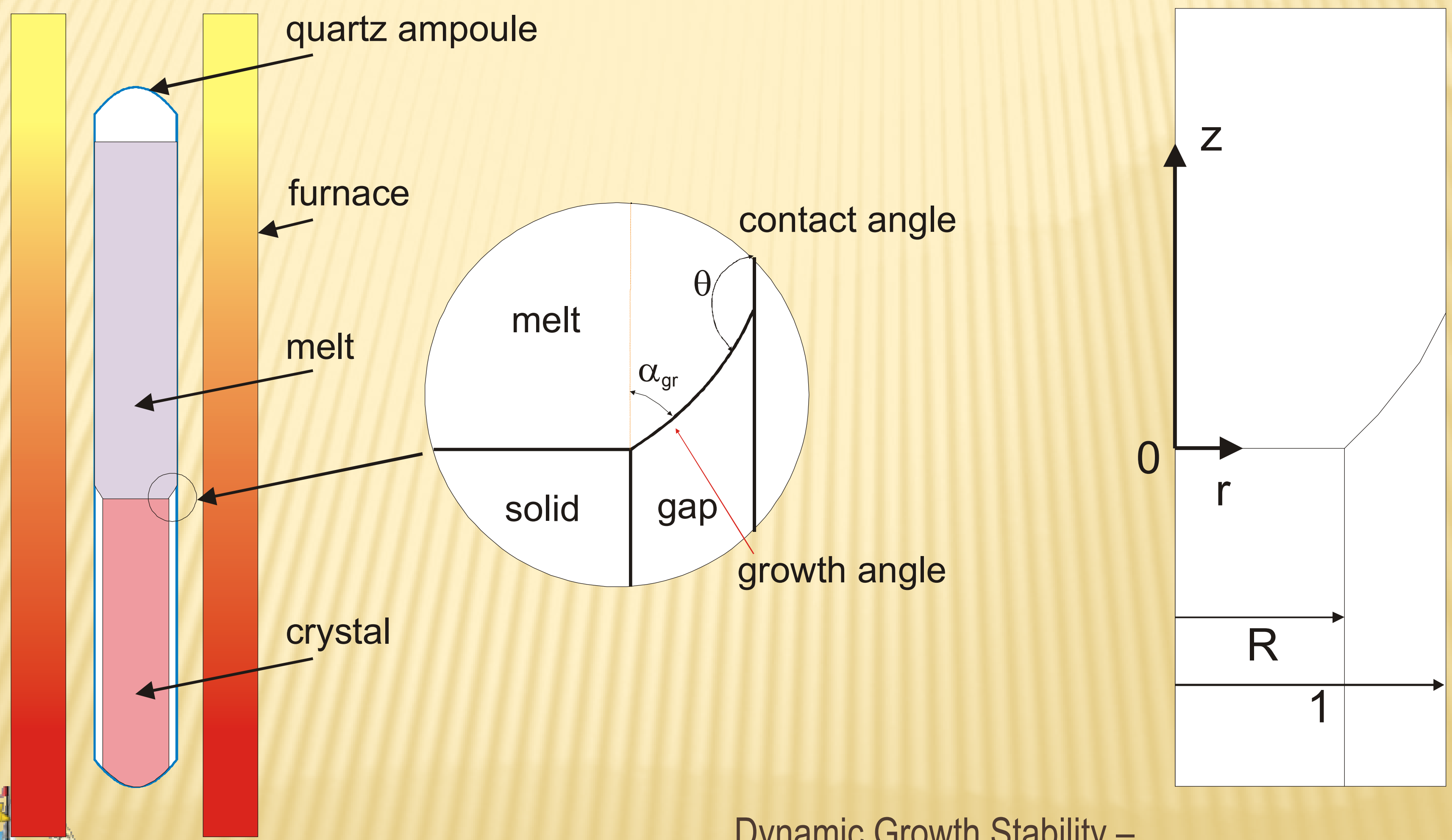
Bridgman crystal growth can be conducted in the so-called "detached" solidification regime, where the growing crystal is detached from the crucible wall. A small gap between the growing crystal and the crucible wall, of the order of 100 micrometers or less, can be maintained during the process. A meniscus is formed at the bottom of the melt between the crystal and crucible wall. Under proper conditions, growth can proceed without collapsing the meniscus. The meniscus shape plays a key role in stabilizing the process. Thermal and other process parameters can also affect the geometrical steady-state stability conditions of solidification. The dynamic stability theory of the shaped crystal growth process has been developed by Tatarchenko [1]. It consists of finding a simplified autonomous set of differential equations for the radius, height, and possibly other process parameters. The problem then reduces to analyzing a system of first order linear differential equations for stability. Here we apply a modified version of this theory for a particular case of detached solidification. Approximate analytical formulas as well as accurate numerical values for the capillary stability coefficients are presented. They display an unexpected singularity as a function of pressure differential. A novel approach to study the thermal field effects on the crystal shape stability has been proposed. In essence, it rectifies the unphysical assumption of the model [1] that utilizes a perturbation of the crystal radius along the axis as being instantaneous. It consists of introducing time delay effects into the mathematical description and leads, in general, to stability over a broader parameter range. We believe that this novel treatment can be advantageously implemented in stability analyses of other crystal growth techniques such as Czochralski and float zone methods.

[1] V. A. Tatarchenko, *Shaped Crystal Growth*, Springer, 1993, pp. 19.

STABILITY OF DETACHED SOLIDIFICATION

K. Mazuruk, University of Alabama in Huntsville
M. P. Volz, MSFC/NASA
A. Cröll, University of Freiburg

DETACHED BRIDGMAN GROWTH



Dynamic Growth Stability –

V.A.Tatarchenko – Shaped Crystal Growth

SYSTEM RESPONSE TO PERTURBATIONS

Linear response of perturbed crystal radius and height

$$\delta \dot{R} = A_{RR}\delta R + A_{Rh}\delta h$$

$$\delta \dot{h} = A_{hR}\delta R + A_{hh}\delta h$$

Stable growth if

$$A_{RR} + A_{hh} < 0$$

$$A_{RR}A_{hh} - A_{Rh}A_{hR} > 0$$

CAPILLARITY PROBLEM

Young-Laplace equation

$$\frac{z''}{\left(1+z'^2\right)^{3/2}}+\frac{z'}{r\left(1+z'^2\right)^{1/2}}=a-b\,z(r)$$

$$a=\frac{\Delta P_m r_C}{\gamma} \qquad b=\frac{\rho g_0 r_C^2}{\gamma} \qquad \Delta P_m=\left(P_{top}+\rho g H\right)-P_{bot}$$

CAPILLARY COEFFICIENTS - THEORY

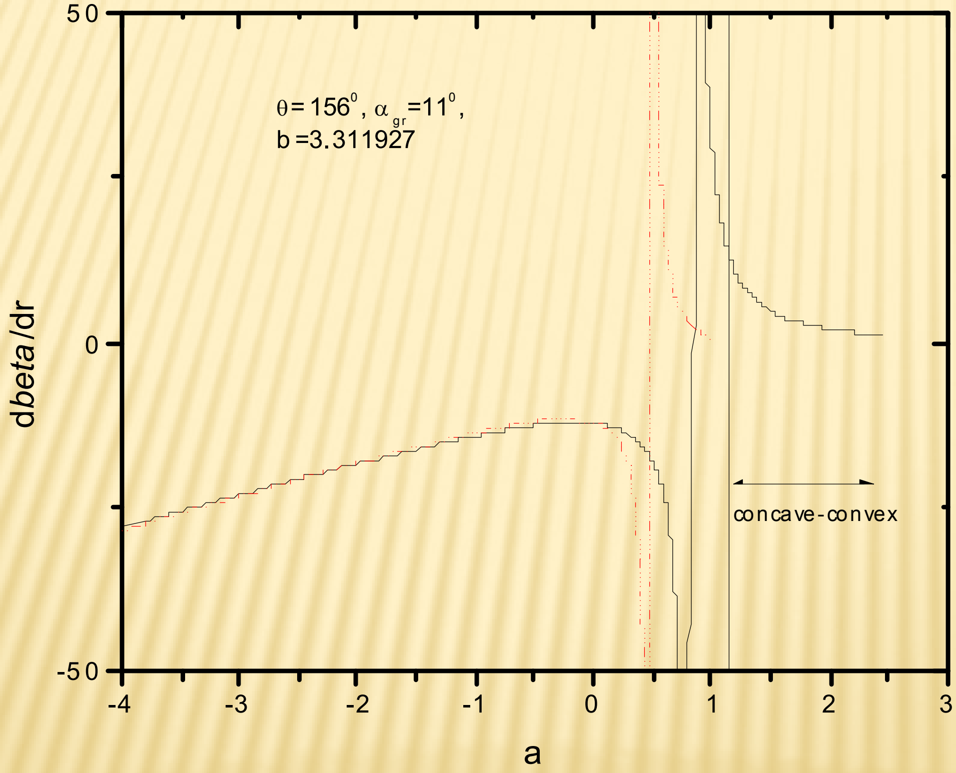
$$A_{RR} = -V\frac{\partial \beta}{\partial R} \qquad A_{Rh} = -V\frac{\partial \beta}{\partial h}$$

V – pulling rate

$$\frac{\partial \beta}{\partial R} = \frac{\left(aR - \cos\alpha_{gr}\right)\sin\left(\alpha_{gr}\right)^2}{R\sin\left(\alpha_{gr}\right)^3 - 1b\left(5 - R\right)^2\left(2 \quad 4 + R \quad 8\right)}$$

$$\frac{\partial \beta}{\partial h} = -\frac{r_C^2 \rho g}{2\gamma}\frac{\left(1 - R^2\right)\sin\alpha_{gr}{}^2}{R\sin\alpha_{gr}{}^3 - b1\left(5R\right)^2\left(2 \quad 4 + R \quad 8\right)}$$

CAPILLARY COEFFICIENTS - NUMERICS



THERMAL RESPONSE - BASICS

Boundary condition at the interface $$V_C L = k_S \frac{\partial T_S}{\partial z} - k_L \frac{\partial T_L}{\partial z}$$

Growth rate $$V_C = V + \partial h / \partial t$$

Height perturbation – Tatarchenko's model

$$\frac{\partial \delta h}{\partial t} = L^{-1}\left(k_S \frac{\partial G_S}{\partial h} - k_L \frac{\partial G_L}{\partial h} \right) \delta h + L^{-1} \underbrace{\left(k_S \frac{\partial G_S}{\partial R} - k_L \frac{\partial G_L}{\partial R} \right)}_{\text{questionable}} \delta R$$

$$\boxed{\delta G_S \neq \frac{\partial G_S}{\partial R} \delta R}$$

ONE-DIMENSIONAL LUMP HEAT MODEL

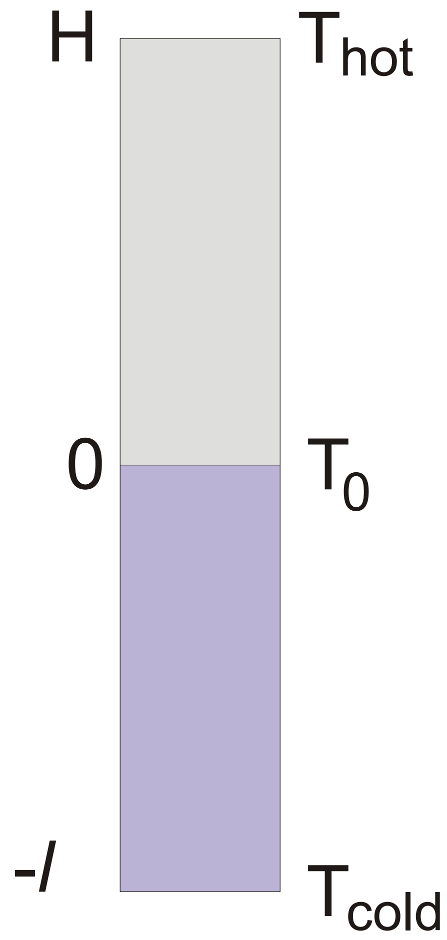
For melt
$$\frac{\partial^2 T_L}{\partial z^2} + \frac{V}{\kappa_L}\frac{\partial T_L}{\partial z} - \frac{\mu_L}{k_L}\frac{2}{r_C}\left(T_L - T_e\right) = 0$$

For crystal
$$\frac{\partial^2 T_S}{\partial z^2} + \frac{V}{\kappa_S}\frac{\partial T_S}{\partial z} - \frac{\mu_S}{k_S}\frac{2}{R + \delta(z)}\left(T_S - T_e\right) = 0$$

$$A_{hh} = -L^{-1}k_L\frac{T_{hot} - T_0}{H^2} - L^{-1}k_S\frac{T_0 - T_{cold}}{l^2}$$

Perturbation of thermal gradient at the interface due to crystal radius variation (convolution):

$$\delta G_S = -\frac{2\mu_S\left(T_0 - T_{cold}\right)V}{R^2 k_S}\int_0^t \delta R(t') e^{-V(t-t')\sqrt{\left(\frac{V}{\kappa_S}\right)^2 + \frac{8\mu_S}{k_S R}}} dt'$$



GENERALIZED RESPONSE

$$\delta\dot{h} = \int_0^t \delta R(t')\,G(t-t')\,dt' + A_{hh}\delta h$$

$$\delta\dot{R} = A_{RR}\delta R + A_{Rh}\delta h$$

Laplace transform solution

$$h(s) = \frac{G(s)\delta R(0) + s\left(\delta h(0) - A_{RR}\right)}{s^2 - s\left(A_{RR} + A_{hh}\right) + A_{RR}A_{hh} - A_{Rh}G(s)}$$

$$R(s) = \frac{\delta R(0)\left(s - A_{hh}\right) + A_{Rh}\delta h(0)}{s^2 - s\left(A_{RR} + A_{hh}\right) + A_{RR}A_{hh} - G(s)A_{Rh}}$$

GENERALIZED RESPONSE CONT.

Tatarchenko model gives

$$A_{hR} = -\frac{2V\mu_S\left(T_0 - T_e\right)}{LR^2 s_0}$$

Our model

$$G(s) = \frac{A_{hR}s_0}{s + s_0}$$

$$s_0 = V\sqrt{\left(\frac{V}{\kappa_S}\right)^2 + \frac{8\mu_S}{k_S R}}$$

Response for the induced perturbation can be studied by analyzing the roots of the following polynomial

$$s^2\left(s + s_0\right) - s\left(s + s_0\right)\left(A_{RR} + A_{hh}\right) + A_{RR}A_{hh}\left(s + s_0\right) - A_{Rh}A_{hR}s_0 = 0$$

MODIFIED STABILITY CRITERION

Conditions for stable growth

Our model

$$A_{RR}A_{hh} - A_{Rh}A_{hR} > 0$$

$$A_{RR} + A_{hh} < s_0$$

$$A_{RR}A_{hh} - s_0\left(A_{RR} + A_{hh}\right) > 0$$

Tatarchenko model

$$A_{RR}A_{hh} - A_{Rh}A_{hR} > 0$$

$$A_{RR} + A_{hh} < 0$$

MODEL APPROXIMATIONS

- Environmental temperature is constant
- One-dimensional lump type approximation
- Capillarity – zero order model – no meniscus motion effects, no triple point effects

CONCLUSION

- Capillarity coefficients display singularity
- Thermal response for the radius perturbation is of the convolution type – this modified model is applicable for other types of shaped crystal growth: Czochralski, Float Zone, etc.